

1-Nitropropane
108-03-2 | DTXSID1020980

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.94×10^{-13} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.95×10^{-1}

Confidence level: 6.92×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1-Nitropropane

Measured: 4.40×10^{-13}

Predicted: 5.94×10^{-13}

Image not found

2-Nitropropane

Measured: 2.60×10^{-13}

Predicted: 3.96×10^{-13}

Image not found

1-Nitrobutane

Measured: 1.50×10^{-12}

Predicted: 1.21×10^{-12}

Image not found

N-Butylnitrite

Measured: 2.72×10^{-12}

Predicted: 1.86×10^{-12}

Image not found

N-Nitrosodimethylamine

Measured: 2.53×10^{-12}

Predicted: 1.27×10^{-12}